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British Crystallographic Association



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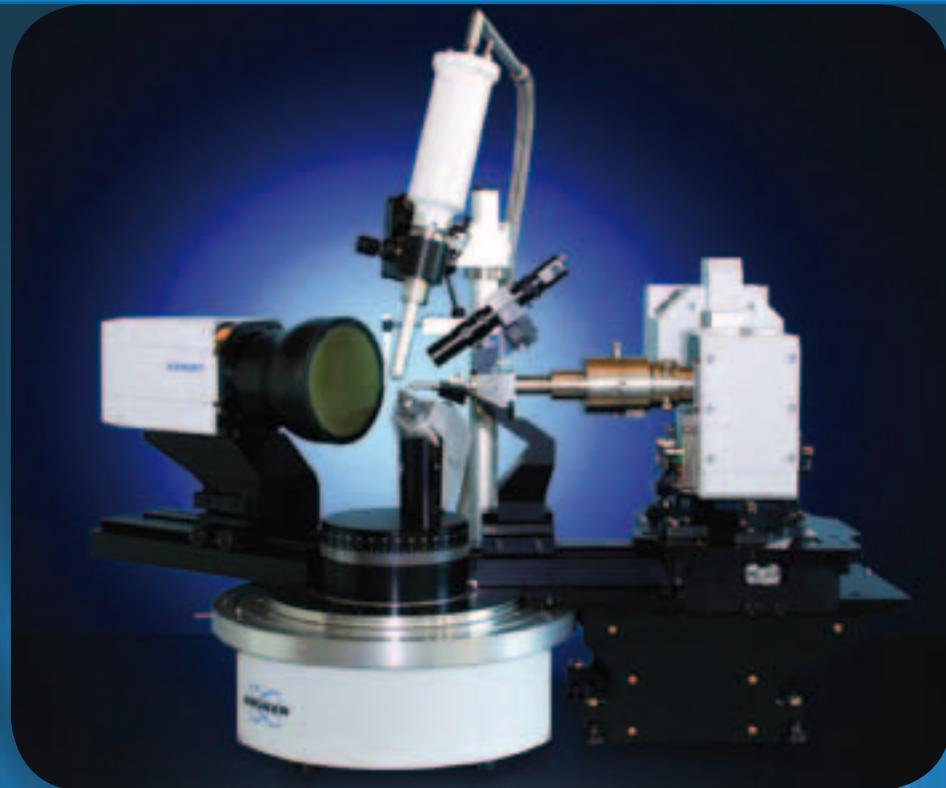


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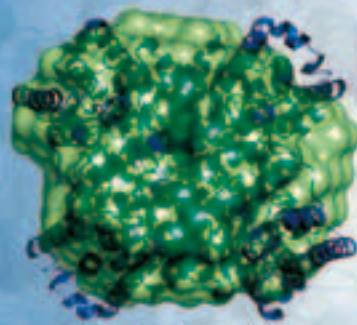
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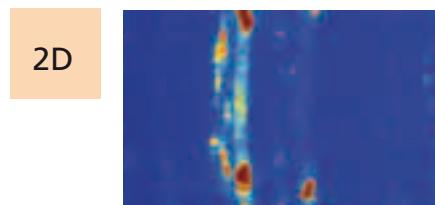
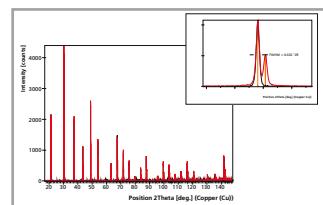
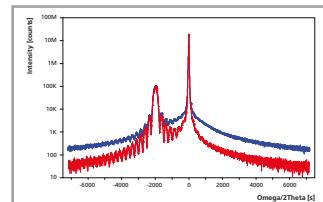


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Crystallography News June 2011

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This month's cover:

*Scenes from
the BCA 2011
Spring Meeting*



From the Editor



THIS issue follows the very successful BCA Spring Meeting that was recently held at Keele University. With their usual combination of intense enthusiasm and professional presentation standards the Young Crystallographers got proceedings off to a very lively start. As planned, the programme for the full meeting featured many joint sessions between BCA Groups and also linked XRD and XRF. In the event these sessions did indeed provide useful opportunities for networking. Despite the uncertain state of the economy we had a full complement of exhibitors, who demonstrated that their product lines are still advancing. Please look at their photographs in this issue. The venue proved to be ideally suited to our needs: all sessions and exhibits were conveniently located in the same building. Participants who wanted a bit of exercise between sessions could explore the green campus, replete with flowering trees, in pleasant spring weather. Keele Hall provided a suitably grand venue for the conference dinner, and both Young Crystallographers and Old Crystallographers demonstrated their impressive terpsichorean skills at the ceilidh. I am grateful to Allan Pang and Joan Schwalbe for most of the photographs illustrating the scenes at Keele.

A fortnight earlier we enjoyed an optimistic CPOSS meeting at UCL on March 30. Beginning with an upbeat assessment by **Sally Price** of progress in the 5th Blind Test of Crystal Structure Prediction, the meeting continued with an impressive set of research results. Details appear in this issue. Thanks to industrial sponsorship this meeting provided proof that there is such a thing as a free lunch.

Of course there is more exciting conference-going in prospect, particularly at the forthcoming 22nd Congress of the International Union of Crystallography in Madrid. While the Early Bird registration deadline will have passed by the time this issue goes to press, regular registration will still be available. The scientific programme and the list of Microsymposia accessible via the IUCr website promise very stimulating presentations.

Our keen anticipation of the 2011 Congress of the IUCr mingles with memories of the 2008 Congress in Osaka, Japan. I am sure that people who were there, like me, were impressed by the courtesy, efficiency and warm friendliness of the Japanese people we met, and were shocked by the appalling tragedy of earthquake and tsunami that hit Japan earlier this year. Among the crystallography laboratories in harm's way were three major facilities: the Photon Factory

synchrotron located about 60 km north of Tokyo, the J-PARC spallation neutron source south of Sendai on the coast, and the adjacent research reactor. Their design specification, providing the greatest protection to the most sensitive parts, is a lesson in good practice. On visual inspection the five protein crystallography beamlines at the Photon Factory appear to have survived unscathed, but the accelerator has suffered significantly: one magnet has toppled and other electronic components have been damaged. Repairs are expected to take several months. At J-PARC a meeting was in progress when the quake struck. The well-drilled participants responded to the shaking by diving under desks, so no one was hurt when the ceiling came down. At J-PARC the tsunami protection did its job, and the massively underpinned experimental hall appears to be undamaged. The dramatic photographs viewable at <http://j-parc.jp/picture/2011/03>StatusEnglish0328.pdf> show the damage sustained by less well-protected ancillary structures, including impassable crevasses that have opened up in the access roads. Fortunately the reactor-based JRR-3 neutron source was undergoing a planned shutdown for maintenance when the quake struck, so no loss of control occurred. Scientists around the world have responded as I expected they would: a fund-raising bake sale at the Stanford Linear Accelerator, an extension of the deadline for Japanese crystallographers to submit abstracts to the Madrid meeting, and offers of beam time at other facilities around the world. Undoubtedly the facilities will be efficiently brought back into operation, but nothing can replace the lives lost; and we extend our heartfelt sympathy to our Japanese colleagues.

Our Directed Assembly Grand Challenge in the use of structural information to design useful materials is continuing to make progress. A series of discussion meetings has been held around the country, and a Network Coordinator has been appointed: Dr. **Jenny Woods**. Information is accessible at www.beyondthemolecule.org.uk. If we are to achieve the difficult goals that have been set, wide-scale communication and collaboration is essential.

Our last issue carried news from the ICDD about the latest round of the Ludo Frevel awards. I suspect that many of us had a vague idea that **Ludo Frevel** was an eminent powder diffractionist but did not know any details. Born in Germany but educated in the USA, he had a distinguished career in industry and with the ICDD. In the latter capacity he established a scholarship fund in 1990, which was subsequently named after him. Over the years he augmented this fund both by fund-raising and by personal donations. Recently the happy news that he had attained his 100th birthday was followed by the sad news of his death. Still, his long and productive life provided evidence that crystallography is good for you!

Carl Schwalbe

BCA Council 2010

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(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website www.crystallography.org.uk

Spring Meeting Registration and Subscriptions:

www.crystallography-meetings.org.uk

Crystallography News June 2011

From the President



DEAR MEMBER

Now the Easter break and the Royal Wedding seem long ago, the lighter days are with us and we can start to anticipate summer activities: crystallographic and otherwise.

The pre-Easter BCA Spring meeting in Keele was very lively and successful, and I am not just referring to the ceilidh here (which for

me was one of the highlights). There were over 280 delegates, with just over 50 of these registered for only one of the days rather than for the whole meeting. There were 90 registered for the Young Crystallographers (YC) symposium, and with other 'older' interested attendees, this meant that the lecture theatre was full for the eclectic mixture of talks which well represented the activity and cutting edge areas of crystallography. It was good to hear a few more Biological Crystallography presentations this year (there was just one in 2010), and I would encourage yet more YCs in this part of our discipline to step forward next year.

The main meeting was seemingly seamlessly organised by Programme Chair **Arwen Pearson** and her Committee: **Trevor Greenhough** (BSG), **Annette Shrive** (BSG), **Stephen Moggach** (CCG), **Hazel Sparkes** (CCG), **Judith Shackleton** (IG), **Kirsten Christensen** (PCG), **David Taylor** (XRF), **Margaret West** (XRF), **Susanne Coles** (YO), **William Lewis** (YO), **Duncan Sneddon** (YC) and **David Allan** (BCA Vice President). We are really grateful to them, and also to the session Chairs, for the time and care they took to make the meeting so memorable. It had a significant number of joint sessions organised by representatives of two or even three of the Groups, and this meant there was much to interest delegates, to the extent that it was often hard to choose which talk to attend. The named lecture in the main meeting this year was the Lonsdale Lecture, which was given by Professor **John Helliwell** from the University of Manchester on the topic of 'The evolution of synchrotron radiation and the growth of its importance in crystallography'. The audience was treated to a marvellous gallop through the history of the use of synchrotrons for crystallography, enlivened by stories from John's wide experience in the field.

The dinner was very well attended and for the first time included dancing to a ceilidh band, which was much enjoyed by those who chose to participate (and also I hope by those encouraged to dance by the President against their better judgement!). The ceilidh was inspired by the observation at the Spring meeting in Warwick last year that the Joint Spring Meeting of the British Society for Cell Biology and the British Society for Developmental Biology were holding their conference dinner in a neighbouring banqueting room, and having a great time at their after dinner ceilidh.

Apart from the efforts of those mentioned above, the success of the Spring Meeting relies heavily on several other factors: the participation of our exhibitors, of whom we had a full house of 23 this year, the organisational skills of Northern Networking with their calm and efficient presence both before and during the meeting, and the helpful cooperation of the local Keele staff. To all those involved we express our appreciative thanks. In terms of facilities, exhibitor space, convenience, logistics and costs, Keele was an excellent venue overall.

In her Introduction to the Programme and Abstract Booklet, **Arwen Pearson** quoted **William Astbury**, who in 1947 wrote: "We need much more cooperation, much more fraternisation, much more encouragement the one of the other, much more sharing of knowledge and much more asking of help." This sees an excellent exaltation to be remembered as a mantra in our daily working lives.

At the BCA AGM in Keele our intrepid and very hard working Treasurer, **Harry Powell**, retired after his three year term. I would like to repeat the thanks of the BCA which were expressed both at the AGM and the Meeting dinner to Harry for the very careful way he has steered and managed the BCA finances, and expertly expedited the change to the CAF Bank. Our new Treasurer is **Andrea Mulholland**, a Biological Crystallographer who has been heavily involved in the Committee of the BSG for many years as both BSG Chair and Treasurer.

According to a scheme agreed in 2009 by Council, we are staggering the election of new ordinary members of Council at one a year, instead of electing a completely new triplet every three years. To achieve this, one Ordinary Council Member kindly stepped down (**Alex Griffin**) and was then co-opted back onto Council, and **Amber Thompson** was elected onto Council.

Several issues arose during the AGM to which Council will give its attention over the coming months. A pressing concern is the falling membership of the Association: we currently have just over 500 members, which is significantly lower than 5 years ago. A challenge was made to the membership attending the AGM to recruit new members and to rerecruit lapsed members. As an incentive to members to help in this drive, the BCA member who recruits the most members (n) over the next year (as long as n>10) will win a free registration to the ECM Meeting in Warwick in 2013. To this end, the membership form now has an additional box asking for the name of the BCA member who recruited the joining member. If each member recruited just one person, we would double our membership and ensure the sustainability of the Association.

The IUCr Congress in Madrid will soon be on us. At it, the BCA will have 5 representatives at the General Assembly. The BCA President, Vice President and Secretary will be present and will attend the meetings, which are to be held on the evenings of Tues 23rd, Wed 24th, Sat 27th and Sunday 28th August (the latter will only be held if required). If any Member is going to Madrid and is interested in attending one of these meetings of the Assembly, please let me know soon, so that we can ensure we are fully represented.

Another notable crystallographic event of the summer will be the CCP4/BCA Protein Crystallography Summer School in St. Andrews from 3-9th September organised by **Garry Taylor** and **Jim Naismith**.

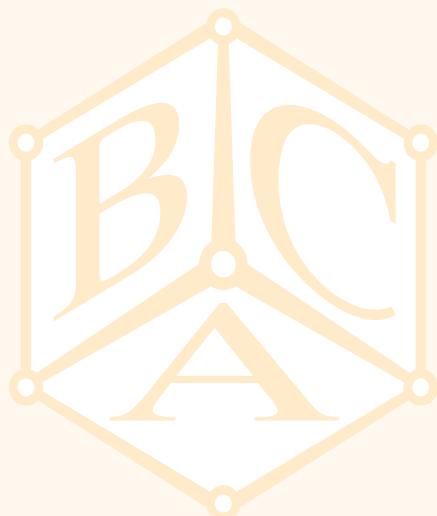
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Elspeth

Puzzle Corner

I have decided to hold the March puzzle over for another three months. I know that March was a busy time for many crystallographers, what with the need to prepare for the BCA meeting and to meet abstract deadlines for other meetings; and I hope that more people may now have time to give it a try. As a reminder, it concerned a banana-loving camel who needed to eat 1 banana every mile to fuel his locomotion. If he starts with a stash of 300 bananas but can only carry 100 at a time, how far can he travel?

(Contributed by Elspeth Garman)



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BCA Annual Spring Meeting 2011

University of Keele 12th-14th April 2011

THE 2011 BCA spring meeting was held at the University of Keele 12th-14th April. As is traditional the Young Crystallographers Meeting occurred before the main meeting on the 11th and 12th April. This year we were also joined by the XRF community who held a workshop on the 12th April followed by scientific sessions during the main meeting.

This well-attended meeting was a great success! Because of the short time interval between the conclusion of the meeting and the copy deadline, this issue will only carry one participant's impression along with reports of the meeting of the Young Crystallographers and the Plenary Lectures. In-depth reports on the Group Sessions will come next time. However, I must depart from editorial standards of fairness and balance to mention one excellent group lecture out of the many excellent lectures that were delivered.

Plenary Lectures

In keeping with the interdisciplinary theme of the meeting, these lectures were noteworthy for broad scope as well as intellectual depth. I am including descriptive notes by **Helge Dorfmüller** in these reports.

The Lonsdale Lecture forms a bridge between the Young Crystallographers' meeting and the main meeting. This year it also served as the BSG Plenary, and **John Helliwell** gave a lecture which successfully addressed all these objectives and held the attention of everyone in this diverse audience.



John Helliwell

He started his lecture by summarizing the stages in the progress of synchrotron radiation (SR) sources through the 1st, 2nd and 3rd generations, and the 4th generation which is under development at the moment. He described his and his colleagues' involvement in the development

With astonishing prescience the Programme Committee scheduled a lecture by **Scott Owens** from the National Nuclear Laboratory on the importance of crystal growth in the nuclear industry. With events at Fukushima fresh in our minds this lecture was particularly well attended. He showed us the importance of an understanding of crystals and crystal formation at all stages of the nuclear fuel cycle, but an example from the end stage was particularly memorable. The early storage ponds for spent fuel at Sellafield were open-air and only covered later. The presence of nearly every element in the Periodic Table arising from radioactive decay over decades, suspended in liquid made highly alkaline to suppress metallic corrosion, to which unquantified but generous amounts of seagull excrement had been added, posed unique challenges in phase identification!

CARL SCHWALBE

of the 3rd generation of synchrotron sources, including the use of undulators to obtain more intense and more focussed beams. He also mentioned that the advances in the light source were accompanied by improvements in the corresponding techniques, for example, in detectors, the use of cryomethods and the reintroduction of the Laue method. John explained how the principle of MAD phasing was developed using two different wavelengths and three measurements to solve the phase problem of protein samples. Afterwards the phenomena of beam heating issues and radiation damage due to cleavage of disulphide bridges were explained, and John showed the first example where he discovered structurally the break-up of a disulphide bridge (1983). Prof. Helliwell further covered the subjects of micro crystallography diffractometers developed by the EMBL and non static crystallography. He then introduced the neutron beamlines to determine the protonation state of side chains using the strong scattering abilities of deuterium in a neutron beam. John ended the Lonsdale Lecture and BSG Plenary with the 'future' of crystallography. Several European light sources are well prepared for further optimisation such as PETRA 3 in Hamburg, Germany with the 'ultimate storage ring' as well as the cutting edge facility at the DIAMOND light source and the upgrade program for nanofocus beams at the ESRF. In this way the x-ray technique steers towards the objective of single molecule diffraction.



Nora de Leeuw and Judith Shackleton (chair)

The topic of the Industrial Group Plenary lecture by **Nora de Leeuw**, "Computational studies of biomaterials", again had wide appeal across the Groups. Already the biomaterials market is \$9 billion in the USA. Natural bone consists of a simple protein phase (collagen I) and a mineral phase (hydroxyapatite). Synthetic equivalents are being sought to treat osteoporosis and improve the compatibility of implants. These large disordered systems provide a challenging research field for modellers. Hydroxyapatite and bioglasses have been treated both by quantum mechanical methods and by classical molecular dynamics (MD); and collagen, by MD. According to MD hydroxyapatite with water on the surface undergoes dissolution of OH⁻ and Ca²⁺. However, the introduction of fluoride causes nearby OH to form O-H...F hydrogen bonds, and the fluoride also helps to anchor Ca. Phosphate-based bio-active glasses promote tissue regeneration and dissolve after repair. Introduction of calcium increases rigidity of the glass. The collagen phase of natural bone is known to consist of 3-strand triple helices, and their association in the bulk material is now better understood.

Judith Howard gave the CCG Plenary Lecture in the all-important Wednesday afternoon slot. She succeeded triumphantly, not only in the presentation of interesting structural chemistry but also in stimulating the audience to remain alert and engaged for the Annual Meeting that followed. Her title was "Intermolecular interactions: their influence on structure and properties".

She described her group's variable temperature X-ray and neutron studies aimed at following structural evolution and the changes in macroscopic properties. These studies often pushed beyond the capabilities of available



Judith Howard

instrumentation and inspired the design of new equipment, including the Fddd diffractometer, the Helix cryostat, the Phenix cryostat and the XPHOS diffractometer for extreme conditions. Research topics covered include LIESST (Light Induced Excited State Spin Trapping) and pressure induced spin transition, conductivity and superconductivity in molecular charge transfer salts, and low melting molecular complexes such as between chloroform and ketones.



Gilberto Artoli



Gilberto presenting his lecture

The last plenary lecture, coming as it does on the morning after the Conference Dinner, needs special appeal to get us out of bed. This year's PCG plenary lecture on "Crystallography in the cultural heritage: personal experiences" by **Gilberto Artoli** certainly provided this appeal by applying modern analytical techniques to ancient objects, including the axe of the famous alpine Iceman. 3-D tomography makes it possible to reconstruct what the layers in badly corroded objects must have been originally. In this way the design of an early Greek astronomical measuring device could be discerned. Texture analysis can reveal the treatment that a metal object has undergone. Comparison of the Iceman's copper axe with 20 other objects of similar age revealed that some had been hammered into shape while others were almost a single crystal that must have been cast in a mould and very slowly cooled. Sicilian baroque blue glass had been a mystery since chemical analysis showed negligible content of Cu and Co, the usual elements responsible for blue colouring in glass. It has now been shown that the Sicilian glass contains Si from flint, K from local plants, and Fe in a very distorted octahedral environment which affects its light absorption. Finally, a source of great embarrassment for museum curators could be cleared up. A collection of ancient flint tools unexpectedly turned blue. X-ray diffraction showed that the underlying structure of the flint was unchanged, but solvent extraction and spectroscopy demonstrated that anti-oxidants in the mats used to cushion the flints had reacted to form dyes.

A newcomer's account of the Spring Meeting

ICDD BURSARY RECIPIENT

As a first year PhD student this was my first BCA meeting and I have to say I was not disappointed! The sessions were all interesting and the speakers excellent. I went to all the talks I was able to go to and I would like to present my thoughts on the talks here.

The first of these was given by Professor **George Sheldrick** who discussed how to handle non-merohedral twinning. He gave a fascinating insight into the practical methods associated with indexing/integrating and scaling non-merohedrally twinned data. This included both emphasis on the need to find a cell which fits most, but not all, reflections in order to index and then to use 3D profile fitting when integrating the data. However, I hope I will be forgiven for not following his final piece of advice to us – to try and grow twinned crystals intentionally as it helps with data collection. This session contrasted well with Dr **Roberto Steiner** who went on to speak about pseudo-merohedral twinning, suggested how to avoid it and gave some useful advice on what to do if it is encountered. This included using additive screens to try to eliminate twinning in the drop, checking all crystals in the drop to see if any are not twinned and, if you are not sure whether twinning is present or not, use the tools available in both Scala (CCP4) and Phenix. Xtriage (Phenix) to examine the data more closely.

The combined macromolecular-chemical crystallography session was very interesting. It began with Professor **Christine Cardin** speaking about a large chemical structure and a relatively small biological structure. The difficulties of large chemical structures are something not widely spoken about as, in my experience, chemical structures are a lot smaller than macromolecular (for good reason!).

However it was the second talk which especially captivated me as it was focused on using a complementary technique to tell us more about the structure – terahertz spectroscopy. Dr **Arwen Pearson** spoke about the limitations in macromolecular crystallography including the problem of radiation damage and a tendency to get low resolution data. Another issue comes when studying the action of enzymes, in that most intermediate forms cannot be trapped and as such are invisible in the crystal structure. Her proposed solution to this was to use terahertz spectroscopy to probe the crystal and deduce the changes in both chemical and structural properties.

On Tuesday night the posters were presented. This gave me the opportunity to talk to a lot of people about my work so far and what we intend to do in the future. I received several very good suggestions for future work which we will try and do. I also found it very useful to have people ask me questions about my work as being able to answer them built up my confidence with speaking. Next year I would like to present a talk at the Young Crystallographers meeting as well as presenting another poster as I found the evening very enjoyable.

On Wednesday the first crystallization session involved the use of very specific crystallization conditions to grow crystals of a certain morphology. Dr **Karen Harvey** spoke about the use of crystals in the film industry and it was fascinating to see how crystals of different sizes and shapes could affect the properties of the resulting film. With large crystals being the most sensitive to light it is important to obtain the correct size distribution for the film being manufactured. For example larger crystals are used in the manufacture of cinema film as this gives a more uniform reaction to light. Additionally, the growth of octahedral crystals giving the $\text{AgX}[111]$ (where $\text{X} = \text{Cl}$ or Br) face is important for the industry as this enhances the light sensitivity and makes a better film. The mechanism of latent image development was also discussed revealing that it is Ag_6^+ which gives the image after a large set of chemical reactions which build up to Ag_6^+ from Ag_2^+ .

A very interesting talk was given by Dr **Scott Owens** on how crystallization is important to the nuclear industry. In this he showed several images of crystal clouds which are encountered in the nuclear pools. Due to the amount of radiation present all of the crystals seemed to have completely different morphologies, as well as showing how difficult it is to form the correct crystals in the fuel rods themselves.

It was the radiation damage session though that I was most interested in as I am doing some radiation damage studies during my PhD. This started with Professor **Elspeth Garman** giving an overview on radiation damage and its effects in macromolecular crystallography. As current synchrotron sources are so bright a crystal can be damaged within seconds of exposure losing vital structural information. She also outlined the different types of radiation damage which can happen. Primary damage is where the crystal directly absorbs the energy from the x-ray beam and, unfortunately, this is a function of the laws of physics so we can do nothing to change it. However, secondary damage is where the radiation produces radicals within the solvent channels present in a crystal. These radicals then go on to damage the crystal. This can be managed in a number of ways. The current routine method of this is to use cryocooling whilst collecting data. As 100K is below the temperature where hydroxyl radicals are mobile this can lower the effect of radiation damage. However, we can also use the program RADDOS to calculate how much radiation a crystal will be able to take without showing significant breakdown. This information can then be used to work out the best data collection strategy for the crystal keeping within the 30MGy limit as suggested by Elspeth Garman.

Dr **Frank von Delft** also gave an interesting talk on radiation damage. In this he gave a very useful set of rules for saying what effect a certain dose of radiation will have on a crystal. At 10MGy the intensity of reflections to 1 \AA will fade by half, at 20MGy the 2 \AA reflections will fade by half and at 30MGy the 3 \AA reflections will fade by half. This is good information to have when considering the best data collection strategy for a crystal.

I was also fortunate to be able to attend one of the XRF sessions. The talks were most interesting and it was great to see the versatility of the technique. **D. J. Bellis** began by talking about how XRF had been used to make a 2D map of the presence of metals in bones from goats as a part of tests for lead in the US. A grid scan of a cross section of bone was taken and this was plotted into a 2D map to show the concentration and distribution of lead in the bone. This was then compared to ICP-MS to validate the results and the comparison was very good. This technique was also used to map iron in the brain of a mouse. **Nick Marsh** also gave a good talk on how XRF was being used to study climate change from the SiO₂ cell walls left behind in lakes by diatoms. Scanning fluorescence microscopy was first used to find contaminants in the samples with XRF then being utilised to look for both major and trace elements and assign these to the contaminants. The abundance of ¹⁶O and ¹⁸O could then be established to give us a record of past climate conditions.

On the Wednesday evening we had the conference dinner and Ceilidh which was great fun! The dinner was excellent and I was awarded a prize for my poster – something which definitely boosted my spirits further! The Ceilidh was a wonderful idea, and the music which was played really made the evening go off with a bang (as did the wine). It was great to get to talk to others about their research in a more informal setting.

The following morning, with blurry eyes, we turned up to the plenary given by Professor **Gilberto Artoli** on the subject of crystallography in cultural heritage, a most interesting session showing how crystallographic techniques can be used to analyse samples from the past including paintings and coins. This was followed by the BSG Young Crystallographers' showcase. I thought this was excellent and it was really exciting to see what fellow students were working on and the techniques they used. I found **S. Tanley's** of particular interest as he was studying the binding of cis-platin and carbo-platin to hen egg white lysozyme as I work with DNA and the mode of binding to DNA is very well known!

YCG Satellite Meeting

THE Young Crystallographers' satellite meeting took place at Keele University on the 11th and 12th of April immediately before the main BCA Spring Meeting. There were 14 talks from young crystallographers spread out in three sessions. The scientific breadth, quality of research and quality of the presentations were outstanding.

The opening plenary presentation by **Matthew Johnson** from GlaxoSmithKline highlighted the work of industrial crystallographers and their role in the development of new products and in R&D. He also explained how the Industrial Group of the BCA hope to bridge the gap between academia and industry.

Henry Wong from the University of Nottingham began the oral presentations by young crystallographers introducing his high

The final session of the meeting was getting more from diffraction data. The first speaker, Dr **M. R. Probert**, gave an interesting talk on the challenges of ultra-low temperature data collection and how some of these had been overcome thanks to the program "masquerade". This masks the diffraction rings given by the beryllium cup used to thermally shield the sample. Next was Professor **Chris Gilmore** discussing electron crystallography. I was intrigued as I had never heard of electron crystallography before. He presented a very interesting talk which focused on how electron crystallography is used and both its merits, that it can be used with an extremely small sample size (<50nm), and its downfalls, that the scattered electron beams lead to secondary scatter eliminating systematic absences! Nevertheless he showed us examples of structures that had been obtained using less than 50 reflections. Whilst these were mostly 2D structures it was still incredible that a structure could be solved with so little data. Dr **David Watkin** then finished off the meeting with an insightful talk on multiplicity of observations (MoO). He covered how it was first encountered, why it is useful and what the data can be used for. It lets us check for self-consistency in the data which can help us reduce systematic error. This is done by measuring the spread of the data. If the spread is large it indicates error but if the spread is small this indicates consistent, low error, data.

And with that the meeting was over. This was my first BCA meeting and I have left it with ideas about how to enhance my own work and new experiments to conduct in the future. The meeting was inspirational – the chance to experience the diversity in both current and past research which great. It was a brilliant 4 days (including the Young Crystallographers meeting) and I am certainly looking forward to next year!

JAMES HALL
UNIVERSITY OF READING

pressure studies on a series of palladium thioether coordination complexes. It was interesting to note the change in the pi-pi stacking interactions of these compounds on the application of pressure.

Susanne Coles (née Huth) from the University of Southampton then talked about the relationship between a series of mono-substituted acyanilides, and how the results from over 250 crystal structures could be used to help with structure prediction using the software package XPac.

Oliver Zeldin (University of Oxford) gave his talk on microPIXE, which can be used to detect different metal ligands in proteins. These metal ligands cannot be easily determined using crystallographic techniques and the high throughput application of this technique was demonstrated.

The fourth talk in this session was presented by **Lauren Hatcher** from the University of Bath, introducing her thermal and photocrystallographic studies on a nickel-nitro complex. To date, this is the first crystallographic study of both thermal and photochemical excitation of a nitro ligand within the same system.

Laura Thompson (University of Birmingham) showed two crystal structures of nicotinamide : succinic acid co-crystals; one solved by single crystal while the other through powder X-ray diffraction.

The first session was completed by a presentation on zeolitic imidazolate frameworks by **Ines Collings** from the University of Oxford. Her talk highlighted the similarities between these frameworks and silicates, and how the framework flexibility alters their mechanical behaviour.

The second plenary was given by this year's programme chair, **Arwen Pearson** from the University of Leeds, who introduced the exciting new developments in trapping and probing reaction intermediates in enzymes with the combined techniques of spectroscopy and X-ray diffraction.

Andrew Jones (University of Glasgow) spoke about the use of Laue neutron diffraction at the ILL to explore hydrogen bonding. His results were complemented by studies using X-ray diffraction and were focused on studying proton migration, proton transfer and proton disorder and examples of all three were given.

Claire Murray (University of Reading) discussed the formation of large multi-nuclear cages from ortho-palladated ligands and central bridging ligands, and their characterisation by single crystal X-ray diffraction and ¹H NMR studies. Variations in reaction stoichiometries, as well as choices in solvents of crystallisation were seen to be vital in the synthesis of expected and unexpected structural analogues.

Miriam Walden (University of Leeds) explained that during the mitosis of Drosophila neuroblasts several molecules are vital in order for the cell division to occur. Through the use of high resolution X-ray crystallography, the structures of the proteins involved in the cell division could be determined.

Nick Funnell (University of Edinburgh) demonstrated how high pressure can be used in crystal engineering to target the formation of specific polymorphs. He also explained by using heat how crystal formation can be achieved inside a high pressure cell.

In line with previous years, a flash poster presentation session finished off the day's activities. All of the young crystallographers who were presenting posters were invited to describe their poster in exactly 30 seconds. In total, there were approximately 30 presented which represents a sizable proportion of the posters presented at the Spring Meeting.

Tuesday's opening session was the official inauguration of the YCG Parkin lecture, which is to be awarded to a young crystallographer to recognise outstanding contributions to promoting science, raising public awareness of science and showing originality in research. **Helen Maynard-Casely**

from the Royal Institution of Great Britain was selected as this year's prize winner for her outstanding public engagement, both during and after her PhD. Helen's talk was a fascinating introduction to her work at the Royal Institution and to her work in communicating science to the wider public, with a particular emphasis on encouraging other people who enjoyed her talk to become involved in the public understanding of science.

The synthesis and investigation of several anil derivatives has been carried out by **Helen Mason** (University of Durham) to examine structure-property relationships in these compounds.

She demonstrated through the change in substituents how the thermo- and photochromic properties can be dramatically altered.

Crystallisation of horseshoe crab serum amyloid P component was described by **Matthew Mold** from Keele University. High resolution diffraction data of the octameric form of the protein were reported, and the future plans to obtain the structure in copper-bound form were discussed.

Daniel Bailey discussed his work with the compound $[PdCl_2([9]aneS_3)]$, which he has shown to convert from a mononuclear complex to polymeric chain when it is pressurized to 44 kBar.

In addition to the structural changes induced, the polymer chain is also found to be intensely coloured. Further pressure studies with the analogous bromo and iodo complexes were also discussed.

Kirsten Christensen from I19 at Diamond Light Source talked about the difficulties in the diffraction of the simple molecule, trimesic acid. The crystal structure is twinned as well as the diffraction pattern containing additional satellite reflections.

The final session of the satellite meeting was a careers development session introduced at the suggestion of the program committee chair, **Arwen Pearson**. **Paul Raithby** from the University of Bath gave a presentation entitled 'The Rocky Road to becoming an Academic' and **David Berry** from AstraZeneca gave his talk on 'Careers in Solid-State Chemistry-Pharmaceutical Development'. It was especially nice to hear from David, as only a few years ago he was giving a talk as a young crystallographer. Both of these talks gave rise to lively debate from the audience and a lot of useful advice was given by both speakers.

Feedback from this meeting was especially good, and the success of the meeting was, in a large part, a result of the fantastic audience participation and the large number of questions from both young and not-so-young crystallographers, perhaps somewhat swayed by the possibility of winning an elusive Diamond Light Source glow stick! This is an important part of any forum and this interaction should be encouraged. Hopefully this will encourage the young crystallographers to ask questions in other meetings.

Prize Winners

Congratulations go to the following winners of awards and prizes:

PCG PANALYTICAL THESIS PRIZE

Stewart Bland (Elsevier)



CCG CRYSTENGCMM PRIZE

Elena Marelli (Reading)



CRUICKSHANK PRIZE

Claire Murray (Reading)



PCG POSTER PRIZE

Jonathan Coome (Durham)



CCG PRIZE

Marc Schmidtmann (Liverpool)



BSG PRIZE

Ivo Tews (Southampton)



YC TALK PRIZE

Oliver Zeldin (Oxford)



CCDC PRIZE

Peter Wood (CCDC)



RIGAKU PRIZE

James Hall (Reading)



CCG INTERNATIONAL TABLES PRIZE

Jasper Adamson (Oxford)



YC POSTER SUMMARY AWARD

Lynne Thomas (Bath)









Spring Exhibi



Exhibitors 2011



News

Young Crystallographers Satellite meeting

THIS year's Young Crystallographers Satellite meeting took place immediately before the main BCA Spring Meeting at Keele University. The meeting was very well attended with the room very nearly at capacity and with some people preferring to stand, setting a high water mark for the YCG satellite meeting. This is a great endorsement for the YCG and the talks this year did not disappoint. Of course, the meeting as a whole offered a great opportunity to catch up with and meet new scientists and it was particularly welcoming to see the vendors attending the poster session on Monday night. At this juncture, the young crystallographers should be encouraged to speak to exhibitors as their support for the spring meeting is very welcome.

This year saw the first Parkin lecture given by a young crystallographer, Dr **Helen Maynard-Casely**. Her talk was extremely entertaining and no doubt will be further mentioned in this issue of Crystallography News. One notable highlight of Helen's talk was the cameo appearance of the chem-moo-stry cow, a creation of the late Dr. Andrew Parkin in partnership with Dr Gordon Barr.

It is the responsibility of the YCG committee to award the Durward Cruickshank Young Crystallographers' Prize to a person who has made an outstanding contribution in any area of crystallography and to the Spring Meeting. This

year, the prize was awarded to **Claire Murray** who gave a talk, presented a poster, organised the poster session and was elected to the YCG committee as deputy-chair during the meeting. She has also been involved with various outreach projects throughout the year.

At the recently held Young Crystallographers Group AGM, a decision had been made to shift the turnover period of the chair by a year in the future in order to avoid the simultaneous

replacement of the "senior" part of the committee: the chair, deputy chair and the secretary. In accordance with this, **Susanne Coles** (née Huth) stood down as chair and was replaced by the now former deputy chair **Duncan Sneddon**. In addition to this, **Arefeh Seyedarabi** as BSG representative, **Claire Murray** as IG representative, **William Lewis** and **Soshichiro Nagano** as Ordinary Members retired from their respective positions. **Claire Murray** was elected to the position of deputy chair and **Soshichiro Nagano** was elected as the new BSG representative.

After a year of vacancy in the webmaster slot, the post is now filled by **Allan Pang**. **Lauren Hatcher** happily

accepted her role as the new IG representative. Four ordinary members were welcomed to the group - **Geoffrey Masuyer, Helen Mason, James Hall, and Robert Young**. **Anna Stevenson** as Secretary, **Peter Byrne** as CCG representative and **Samantha Callear** as PCG representative retained their respective positions for one more year.

In her final Chair's Report, **Susanne Coles** (née Huth) discussed the preparation of the YC satellite for the BCA Spring Meeting, and the committee's role in this. The plenary sessions for the BCA Spring Meeting were reduced from three to two in order to accommodate the Parkin Lecture. In addition, over the last six months, funding for the YCG has also been discussed. Several funding bodies were approached by the committee but unfortunately this was not very successful. In line with the money matters the secretary of the committee, **Anna Stevenson**, reported opening of the new bank account for the YCG. NatWest was chosen for their flexible management under multi account holders and the large number of branches throughout the country. The most urgent agenda upon the committee remains in securing a source of funding. In the coming year, the committee will explore sources of funding in order to solidify the position of the YCG within the BCA.

Finally, the YCG website has recently been revamped and is currently undergoing a radical transformation in the hands of the new webmaster. The site can be found at <http://ycg.crystallography.org.uk/> and is well worth a visit. The long term plan for the website is to make it interactive and accessible to many young crystallographers, as such, members are encouraged to contribute articles and news on the area of their research. The site is open for comments and suggestions, please do not hesitate to contact the YCG webmaster, **Allan Pang**.



Claire Murray



Allan Pang

BCA Accounts 2010

The British Crystallographic Association Summary Financial Statements for year ended 31 December 2010

Examining Accountant: R A Young, BSc, FCA
The Young Company, Ground Floor, Unit 2b Vantage Park,
Washingley Road, Huntingdon, Cambridgeshire PE29 6SR

These are consolidated accounts based on the unaudited financial statements and include the BCA, BSG, IG, CCG and CCG School funds, expressed in pounds sterling (£)

INCOMING RESOURCES:

	<u>2010</u>	<u>2009</u>
Grants and sponsorship	8,072	5,800
Donations	656	8,067
Annual conference (5)	99,925	99,572
Meetings of groups	8,452	21,254
Crystallography News	10,828	18,710
Membership Subscriptions	9,047	18,640
Investment income	4,637	3,981
Interest received	146	851
TOTAL INCOME	141,763	176,875

EXPENSES:

	<u>2010</u>	<u>2009</u>
Direct charitable expenditure (2)	121,397	145,681
Trading stock written off	-	493
Management and administration (3)	30,925	34,233
TOTAL EXPENDITURE	152,322	180,407

	<u>2010</u>	<u>2009</u>
NET (EXPENDITURE):	(10,559)	(3,532)
Unrealised gains (losses) on investment assets	5,369	4,942

NET MOVEMENT IN FUNDS

	<u>2010</u>	<u>2009</u>
Balances brought forward at 1 January	200,191	198,781
Balances carried forward at 31 December	195,001	200,191

ASSETS:

	<u>2010</u>	<u>2009</u>
Fixed assets	5	5
Tangible assets	109,933	59,555
Total	109,938	59,560

Current assets

	<u>2010</u>	<u>2009</u>
Stock	-	-
Debtors	14,370	5,446
Cash at Bank	95,961	154,277

	<u>2010</u>	<u>2009</u>
Total	110,331	159,723

LIABILITIES: amounts falling due within one year (24,548) (18,212)

LIABILITIES: amounts falling due after one year (720) (880)

NET ASSETS 195,001 200,191

INCOME FUNDS:

	<u>2010</u>	<u>2009</u>
Restricted funds (4)	103,582	101,878
Unrestricted funds (4)	91,419	98,313
Total	195,001	200,191

NOTES TO THE SUMMARY FINANCIAL STATEMENTS

1. ACCOUNTING POLICIES.

These summary statements are based on financial statements which have been prepared under the historical cost convention, with the exception of investments which are included at market value. The financial statements have been prepared in accordance with the Statement of Recommended Practice, "Accounting and Reporting by Charities" published in March 2005 and applicable accounting standards.

All incoming resources are included in the Statement of Financial Activities when the charity is legally entitled to the income and the amount can be quantified with reasonable accuracy. All expenditure is accounted for on an accruals basis and has been included under expense categories that aggregate all costs for allocation to activities. Investments are stated at market value at the balance sheet date.

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives.

2. DIRECT CHARITABLE EXPENDITURE

	<u>2010</u>	<u>2009</u>
Subscription to International bodies	9,737	9,875
Annual conference (5)	87,659	91,760
Meetings of groups	6,540	5,139
Crystallography News + Newsletters	14,244	18,129
Course fees and accommodation	-	15,558
Grants and sponsorship	2,180	720
Awards & bursaries	287	2,250
Arnold Beevers Bursary Fund	750	2,250
Total	121,397	145,681

3. GOVERNANCE

	<u>2010</u>	<u>2009</u>
Administration fee	19,119	18,167
Administration expenses	2,159	9,017
Accounting fee	4,500	4,113
Insurance	470	432
Bank and security charges	2,656	664
Special Interest Group Administration	886	637
Council members' expenses	1,135	1,203
Total	30,925	34,233

The full BCA accounts for 2010 are available as an e-mail attached file from the BCA administrative office.

4. STATEMENT OF FUNDS	Brought Forward	Incoming Resources	Transfers Resources Expended	Gains/ (Losses)	Carried Forward
UNRESTRICTED FUNDS					
General Fund	98,313	130,166(141,679)	(750)	5,369	91,419
RESTRICTED FUNDS					
IUCr bursary fund	30,231	-	-	-	30,231
Arnold Beavers bursary fund	11,608	30(750)	750	-	11,638
Dorothy Hodgkin prize fund	8,642	30	-	-	8,672
Chemical group teaching school	18,009	-	-	-	18,009
Chemical group fund	3,791	2,570(2,806)	-	-	3,555
Industrial group fund	11,359	7,336(4,357)	-	-	14,338
Biological Structures group fund	16,488	1,601(2,730)	-	-	15,359
Durward Cruickshank fund	1,750	30	-	-	1,780
Subtotal	101,878	11,597 (10,643)	750	-	103,582
Total of Funds	200,191	141,763(152,322)	-	5,369	195,001

5. Spring Meeting 2010	
Warwick University	
INCOME	
Registration	77,272
Exhibition	21,653
Bursaries	1,000
Total	99,925
EXPENDITURE	
Accommodation & Meals	25,983
Facilities	15,235
Catering	11,481
Social Event	5,780
BCA Speakers Expenses	1,031
Refunds	685
Abstract Book	4,708
NNE Fee	13,876
Administration	4,842
Printing & Stationery	1,142
Young Crystallographers	2,896
Total	87,659
TOTAL INCOME	99,925
TOTAL EXPENDITURE	87,659
MEETING SURPLUS	12,266

All the transactions for the 2010 Spring Meeting were made through the BCA account, and consequently these detailed meeting accounts are reported as part of the BCA financial report

Treasurer's Report 2010

This was a busy year for the BCA and its constituent groups. Overall we had a deficit of £5,190 during the year ended 31 December 2010, and the Association has no material guarantees or commitments which could affect its future solvency.

The general fund had a deficit of £6,894 after an increase of £5,369 in the value of the investments, but the reserve funds

operated by the Groups and the School had an overall surplus of £1,704. The income from our investments brought in £4,783 this year.

The major risks to which the Association is exposed are with regard to the cost of the Spring Meeting and its effects on the Association's major reserves. To mitigate those risks the Association has all its investments placed with an independent professional management company. Our investment portfolio was valued at £109,933. Bank interest rates are at historically low levels, so income from interest is substantially lower than in previous years. In an attempt to mitigate this, the Association has moved part of its reserves from cash at the bank into investment trusts (£25,006) and shares (£20,003 from the IUCr Bursary fund, equally between Royal Dutch Shell and GlaxoSmithKline). The Council's review of the reserves indicates that we should always be striving to generate more income to enable us to plan and encourage even higher levels of educational and scientific activity.

The Young Crystallographers' symposium before the Spring Meeting in Warwick was well attended and appreciated, and sponsors were generous in their support too. Four Arnold Beavers bursaries were awarded to attendees at the Spring Meeting, and another four were awarded by commercial sponsors. No applications were received for the ECM in Darmstadt or other suitable International meetings. The bursary fund for the IUCr is not required by the organizers of the meeting in Madrid in 2011, so a proportion of the fund has been put into medium term investments. The organizers of the IUCr meeting in Montreal in 2014 have

indicated that they will not require the monies. The Association has decided that it would be possible to offer the fund to European meetings on the same basis as offered to IUCr meetings.

Crystallography News has made a substantial loss this year from income of £10,828. Renewed efforts are required to increase revenue from advertising, but, as always, the BCA thanks its advertisers and sponsors who have continued to generously support our activities. There was a welcome surplus from the Spring Meeting.

Subscriptions to international bodies were £9,737, covering our membership of the IUCr at the five-vote level and also our subscription to the European Crystallographic Association. Administration costs, including expenses, are £21,278. The online payment facility for Group meetings has been utilised by IG this year. The expertise and hard work of Northern Networking Events Ltd is very much appreciated.

Membership income is down by £9,593 this year. This is partly due to lower membership numbers and partly to late payment of Corporate membership. Nothing was received from the Inland Revenue in Gift Aid this year but this should amount to about £3,000 in 2011.

This is my final report as Treasurer. I would like to thank everyone who has helped me in my role over the last three years, in particular the other Officers, members of Council, Gill, David, Jennifer and the team at Northern Networking Events, and our accountants Bob Young and Ray Philpott at The Young Company for all their help throughout the year.

Harry Powell
Treasurer

Central Facility News

IN the previous issue of Crystallography News we completed our initial tour of Diamond Light Source with the intention of turning our attention to the ISIS neutron spallation source. Before we do so, however, it should be mentioned that shortly after the previous article was written the Science Minister, David Willetts MP, visited both Diamond and ISIS on the 14th of March to mark the official inauguration of Diamond Phase III beamline construction and to announce the funding for the Phase II construction of new instruments for Target Station 2 of ISIS. These are crucially important milestones for the future development of both facilities and offer security for their operation and support for the foreseeable future.

These funding announcements come in the context of the changing role of the former Harwell Laboratory. Those of you who have visited either Diamond or ISIS recently may have noticed that the main entrance of what was the Harwell Laboratory has undergone some significant changes. The security lodge has been removed, as the site is gradually being opened up for less restricted access, and this has been accompanied by the erection of signs bearing the new

arrangement in place the site will be developed to host both established and start-up technology companies as well as research organisations. For example, the International Space Innovation Centre has recently been officially opened, in close proximity to the European Space Agency's new UK offices. Further information can be found on the Harwell Oxford web pages (www.harwelloxford.com) including some indications of how the continuing development of the site is envisaged.

For those of you who might be interested in the history of the Harwell Laboratory there is an excellent illustrated book, *Harwell: The Enigma Revealed* by **Nicholas Hance OBE**, which charts the transformation of the site from the time before the arrival of the RAF and the creation of the WWII airfield, through the years that the site was developed into a nuclear laboratory, and up to the present period with the rejuvenation of the laboratory into a science campus. Remnants of the airfield are still visible, particularly in aerial photographs.

Next time, as promised, we will visit ISIS and have a look at the instruments that are of particular interest to crystallographers and how some of them have been developed during the recent long shutdown.



"Harwell Oxford" name for the entire site. This re-branding marks a joint venture between the Science and Technology Facilities Council, the UK Atomic Energy Authority and the Goodman international property group. The objective of this public-private collaboration is to establish a world-leading location for science, technology and business. With this

An aerial view of the Harwell campus, taken by the author in 2007, from a glider. The straight road in the centre of the image, Fermi Avenue, marks the boundary between the Rutherford Appleton Laboratory, on the left (South side) of the road, and the former Harwell Laboratory, on the right (North side) of the road.



ICDD celebrates anniversaries

ICDD was established in 1941 as a non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of crystalline materials. As we celebrate our 70th anniversary, we reflect on our founder's visions to serve as an organization dedicated to diffraction technology and education. From handwritten entries to data cards, keypunch cards, magnetic tape, CDs and DVDs, and now access via the Web our dynamic organization continues to evolve along with the community that it serves. We will continue to be the world center for quality diffraction and related data. We will continue to promote the application of materials characterization methods in science and technology by providing forums for the exchange of ideas and information.

70th Anniversary Servicing the Scientific Community

60th Denver X-ray Conference

25th Anniversary of Powder Diffraction

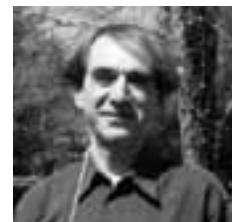
ICDD Announces 2011 Fellow & Distinguished Fellow Award Recipients



Brian O'Connor



Richard C. Bostwick and Tom Blanton (ICDD Chair)



Lawrence Bernstein

THIS year, the Board of Directors recognized **Brian O'Connor**, Curtin University, Perth, Western Australia as the 2011 Distinguished Fellow. This award is given to a member who has given long and meritorious service to the ICDD.

The ICDD awarded two ICDD Fellows at the 2011 Annual Meetings. This award recognizes individuals who have devoted their time and talent beyond what is normally expected of a member. Recognized for their leadership in a noteworthy ICDD activity, the 2011 ICDD Fellows are: **Lawrence Bernstein**, Terrametrix, CA and **Richard Bostwick**, SPEX SamplePrep, NJ.

Data analysis tools now available in Mercury

CCDC are delighted to announce that statistical analysis tools are now provided within Mercury. These tools enable straightforward visualisation and analysis of ConQuest substructure searches where geometric parameters (e.g. bond lengths, angles, torsions etc) have been defined in the query. This functionality replaces that previously provided in Vista, but inclusion within Mercury allows an interesting value of a geometric parameter to be highlighted and immediately

visualised on the molecular diagram. New capabilities include augmentation of the 2-D scatterplots from Vista with colour for the dots, allowing values along a third dimension to be expressed by the colour code.

These new facilities are available for CSD System licence holders. Whether or not they are licence holders, researchers at UK universities can access the new Mercury via the Chemical Database Service at Daresbury.



Meeting Reports

CPOSS Open Meeting, 30 March 2011

THE detailed and informative slides shown at this meeting are accessible on the website www.cposs.org.uk.

Sally Price opened the meeting by reporting the results of the 5th Blind Test. She began by reminding us that crystal structure prediction (CSP) is expected to come up with the most thermodynamically stable structure. The test structures based on single crystal data with limited Z', no disorder and defined growth conditions are likely to comply. Of the 6 structures in the current test, two were small and (fairly) rigid, one had some flexibility, one involved an ion pair, and (in this test for the first time) one was large and very flexible and one was a hydrate with other known polymorphs. Although each structure was correctly predicted by at least one group (provided proton positions were ignored for the hydrate), no method was successful for all targets. She outlined why the organic solid state poses such a challenge to theoretical modelling of relative crystal energies.

Colin Groom presented a panoply of techniques for the avoidance of industrial problems from polymorphism. The reason for the well-known disaster suffered by Abbott Laboratories with ritonavir, where the adequately soluble Form I gave way to the excessively stable Form II, can now be understood. The method of propensity analysis developed at CCDC shows that Form I has two hydrogen bonds that occur rarely while all hydrogen bonds in Form II have higher probability. Participation is also important. For instance, the OH group can form one hydrogen bond either as donor or acceptor, or two hydrogen bonds acting as both. Because three polymorphs of temozolomide all show good propensity and participation, a more stable polymorph is unlikely to be found. The CSD can also give warning of unusual geometry. Rotigotine, a dopamine agonist, showed no polymorphism during development but subsequently changed to a new less bioavailable polymorph. The original form exhibited an unusual torsion angle, which changed by about 100° to a more usual value in the new form.

Colan Hughes changed the focus away from crystallography, showing how solid state NMR can provide valuable information about crystallization in situ. Good sensitivity and time resolution are required if we are to detect the earliest solid particles. To be able to discriminate between polymorphs it is essential to have at least one distinctive peak. The choice of an optimal experimental setup has enabled these prerequisites to be fulfilled in a study of glycine. If 6 M ¹³C₂-glycine is recrystallized from water, only the α polymorph forms; but in D₂O the α -glycine subsequently transforms to the γ polymorph.

Terry Threlfall concluded the morning session with a clear explanation of 1st- and 2nd-order transitions followed by

an exposition of some puzzling experimental results. He enunciated the thesis that classical polymorph transitions can only be first order and discontinuous. The broad transitions that often are observed can be attributed to slow kinetics. Truly continuous second order transitions require a second component. Transitions between low-, room- and high-temperature forms of d,L-norleucine have now been shown to involve only chain slippage and chain rotation. The transition that lies below room temperature is difficult to observe; it typically occurs at -10° to -20°C in Southampton but +10° to +20° in Innsbruck! Another surprising phenomenon involves 2'-nitrobenzaldehyde-2,6-dichlorophenylhydrazone, which has an unstable red form and a stable yellow form. Their structural difference is supramolecular not molecular, involving changes in π -stacking not configuration or tautomerism. Acetaldehyde phenylhydrazone has an intriguing transition when a low melting form is converted to a high melting form by exposure to ammonia and changed back by exposure to acid vapours.

After lunch **Kieran Hodnett** from the University of Limerick told us about the role of transformations in pharmaceutical crystallization. He pointed out that this is a particularly important topic for Ireland since 50% of Irish exports come from the pharmaceutical industry. He defined solution mediated polymorphic transformation as a reconstructive transformation in which the metastable form dissolves, and the stable phase nucleates and grows from solution. He illustrated the process with a striking video that resembled wildlife photography of parasitic grubs burrowing into the body of a caterpillar. On the surface of a large crystal of Form V sulfathiazole small crystals of Forms II and IV nucleate, growing inwards as the original crystal dissolves and eventually taking its place entirely. Forms II and IV have similar atomic layers, and FII can grow epitaxially on FIV.

Chris Pickard returned to the theme of NMR, seeking a "Bragg's Law" for solid-state NMR. In crystallography the inverse problem relates experiment (Bragg peaks) to structure with the aid of theory. The experimental NMR data include shielding, EFGs and J-coupling. The theory may be interpolative (e.g. human expertise or semi-empirical computations) or extrapolative and predictive (first principles or ab initio). Density functional theory provides a way to generate structures that are good to 1-2% and chemical shifts that match experiment to 2% of the shift range. However, this is an "inverse lottery", where you usually win modestly but occasionally lose badly. The high quality data generated by NMR provide an incentive for further improvement of theory.

Finally, under the topic of "Experimental screening and



characterization of solid forms" **Alastair Florence** presented an EPSRC initiative aimed at the ability to manufacture the rationally selected most appropriate physical form. He illustrated it with the forms of creatine, which has sales of around \$400 million as a nutritional supplement in the U.S. Changes in temperature and humidity bring about changes between forms I, II and the monohydrate. The Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation (CMaC) has a budget of £5 million over 5 years. The programme sponsors

the formation of networks and convenes annual meetings. Technology Innovation Centres have been established at UK universities. Further information can be obtained from linda.wallace@strath.ac.uk

A well-attended poster session prompted additional discussion, which was enabled to continue at a bar nearby.

CARL SCHWALBE

Durham School Report



Participants in the 13th Durham School, photographed by Mr Paul Sidney, from the Durham University, School of Biological & Biomedical Sciences, Photographic Unit

THE 13th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis was held at van Mildert and Trevelyan Colleges at the University of Durham between 26th March and 3rd April 2011. The aim of this biennial School is to present the principles of crystal structure analysis using a mixture of lectures and small group tutorials.

The emphasis of the School is on single crystal diffraction, though the majority of topics covered are relevant to all areas of crystallography. We began with the basic mathematical tools used in crystallography, including vectors and matrices, Fourier transforms and symmetry. Topics then followed the course of a typical structure determination: data collection in the lab and at central facilities, solution of the phase problem and Fourier methods, refinement and the analysis and validation of results, including the use of crystallographic databases. Specific lectures were devoted to the frequently encountered problems of

Meeting Reports (Cont.)

disorder, twinning and modulation. As our aim is to teach underlying theory rather than use of specific software packages, the tutorials took the form of paper-based, rather than computer, exercises. Evening activities included a particularly challenging bar quiz and some quite remarkable student presentations, one of which is on its way to becoming a YouTube sensation and compulsory viewing for synchrotron users (<http://www.youtube.com/watch?v=D282Q8AZmFc>).

80 participants attended the School. The majority came from UK universities, although 25% came from overseas. The lecturing team consisted of: **Bill Clegg, Roy Copley, Lukas Palatinus, Simon Parsons, Devinder Sivia, Amber Thompson, David Watkin and Pete Wood.** We are extremely grateful to the dedicated team of tutors: **Birger Dittrich, Francesca Fabbiani, Andrés Goeta, Ross Harrington, Steve Moggach, Iain Oswald, Mike Probert, Hazel Sparkes, Amber Thompson, Claire Wilson and Pete Wood**, most of whom had been students and/or tutors at the School in previous years. Particular thanks go to **David Watkin**, who is retiring this year having been involved in the Crystallography Schools since they began in 1987, and to **Roy Copley, Lukas Palatinus, Birger Dittrich, Francesca Fabbani and Iain Oswald** who joined the lecturing and tutoring teams for the first time this year.

Special thanks also go to **Judith Howard, Andrés Goeta and Hazel Sparkes** for all their hard work with fund raising and local organization, and to **Amber Thompson** who coordinated the production of the course notes. It is important too to acknowledge our sponsors for the financial support provided: DIAMOND, BCA/CCG, IUCr, Cambridge Crystallographic Data Centre, Bruker, Agilent Technologies,

FROM March 26 – April 3 around 80 young crystallographers, primarily PhD students and recent postdocs, ventured up to the University of Durham to participate in the 13th BCA/CCG Intensive Teaching School in X-ray Structure Analysis. The school attracted many students across a range of British and European universities and facilities, as well as a wide range of faculties including chemistry, physics materials science and biology.

The course dutifully led the students through the maze that is crystallography. The lectures and tutorials provided a theoretical context for the entire crystallography experiments from preparing a crystal through data acquisition, solving the initial structure of a crystal, refining the data and publishing the results. Twinning was also discussed and a practical disorder workshop was held. Although there were long hours and a large amount of information the lecturers and tutors managed to keep an up-beat mood and patiently answered all of our questions, no matter how stupid!

Oxford Cryosystems, Rigaku and Chemical Computing Group.

The next School is scheduled for April 2013.

SIMON PARSONS
SCIENTIFIC DIRECTOR



Hazel Sparkes

In addition to the classes there was a pub quiz aptly run by **Stephen Moggach** and **Peter Wood**, which tested both crystallographic and general trivia knowledge, and with a prize of chocolates no one could resist! On the penultimate night it was also the students' turn to do some presentations; although possibly not as informative as some of the lectures, they were very entertaining including some guest appearances from various lecturers turned up in many disguises. The course finished with a formal dinner at Van Mildert College which had provided excellent accommodation and food all week.

On behalf of the students we would like to thank all the lecturers and tutors. Furthermore a special thank you to the organising committee, without whom this wonderful school would not have been possible.

SVEN SYLVESTER

BCA X-Ray Structure Analysis Report:

I attended the BCA/CCG Intensive Crystallography course with some feelings of trepidation.

This may have been in part due to the mention of Intensive in the title, the prospect of a full schedule of lectures, and the epic journey to Durham, thanks in part to the signal failures that shut down the entire northern rail network, and caused me to have to get the bus from York. However I had a great experience at the School. The lectures were all incredibly informative, and entertaining as well. The tutorial questions, and more importantly the mathematics, weren't too horrendous in the end, and all the lecturers and tutors were helpful and brought us back when we wandered too far from the correct answers. It was great to meet others from a diverse set of disciplines and institutions, PhD students and postdoctoral researchers from universities home and abroad, and staff from central facilities. We were able to discuss the different research activities people were involved in, seeing how crystallography is being employed in a vast range of chemical situations and share ideas and techniques with each other. There were still plenty of opportunities for socializing, including a taxing pub quiz,

packed with obscure questions, and my team was slightly disappointed not to have won, especially as we had **Bill Clegg** gifting us the answers in the Crystallography round. There were memorable presentations, which are already making the rounds on YouTube, in one case offering advice on how to survive long hours stuck at central facilities, others describing the horrendous prospect of a future world without crystallography, and impressive singing of The Rhyme of the Ancient Crystallographer. Mid week we were able to escape for the afternoon to Durham city centre, and managed a visit to the Castle and Cathedral, although we sighed slightly when the symmetry of the building was pointed out to us on the tour. Overall I feel I really benefited from the experience, having a deeper understanding of the theoretical basis of diffraction, a greater appreciation of the skills of pre-computer generation crystallographers, and hints and tips for structure solution and refinement to take back and implement in my own research. We were also provided with a comprehensive set of lecture notes for when we encounter difficulties in the course of our research.

ISABELLE KIRBY

THE material in the course takes you through all the steps in solving a crystal structure from picking your crystal right up to structure validation and the teaching is of the highest standard. Importantly the first couple of days were spent bringing everybody up to speed on the mathematics and fundamental crystallography required to get the most out of the course. This was great for newcomers to crystallography such as myself and, although it took some time, I eventually got my head around matrices! The informal nature of the lecturing throughout the course provided a relaxed and entertaining learning environment and the lecturers were ever approachable with any queries.

Within the school we were split into a number of smaller tutor groups and each was assigned an experienced crystallographer as a tutor. In my opinion this was the best point about the course. It allowed us to take on set problems from each module as a group with unhesitating help from the tutor. These sessions ensured that no one was left behind.

In addition to the obvious academic advantages of the course it was also great for networking with people who share your research interests. Although the lectures took up the majority of the time, evenings gave an opportunity to relax in the bar and get to know each other. One afternoon midweek is also allocated as free time to giving us the much needed opportunity to recharge our batteries and offering the chance to explore Durham city or other nearby places.

I went to the crystallography school as someone who could mount a crystal and press go. I'm now in a much greater

position to question and influence what is going on at each stage and deal with more complicated structure solutions for which I give great credit to the course and all of its lecturers!

TOM ROBINSON



Meetings of interest

Further information may be obtained from the websites given. If you have news of any meetings to add to list please send them to the Editor, c.h.schwalbe@aston.ac.uk. Assistance from the IUCr website is gratefully acknowledged.

1-4 June 2011

2011 North American Solid State Chemistry Conference, Hamilton, ON, Canada.
<http://www.brockhouse.mcmaster.ca/news-events/details/23-2011-north>

2-12 June 2011

The Power of Powder Diffraction, Erice, Italy.
<http://www.crystalerice.org/Erice2011/2011pd.htm>

2-12 June 2011

Electron Crystallography: New Methods to Explore Structure and Properties of the Nano World, Erice, Italy.
<http://www.crystalerice.org/Erice2011/2011ec.htm>

6-7 June 2011

XDL 2011 Workshop 1: Diffraction Microscopy, Holography and Ptychography using Coherent Beams, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

6-10 June 2011

TXRF2011. 14th International Conference on Total Reflection X-ray Fluorescence and Related Methods, Dortmund Germany.
<http://www.txrf2011.org>

6-10 June 2011

Fundamentals of X-ray Powder Diffraction, International Centre for Diffraction Data, Newtown Square, PA, USA.
<http://www.icdd.com/education/xrd.htm>

7-17 June 2011

Neutron Instrument Design School, Lund and Simrishamn, Sweden.
<http://ess-scandinavia.eu/nids>

13-14 June 2011

XDL 2011 Workshop 2: Biomolecular Structure from Nanocrystals and Diffuse Scattering, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

13-15 June 2011

Materials Characterisation 2011. Fifth International Conference on Computational Methods and Experiments in Materials Characterisation, Kos, Greece.
<http://www.wessex.ac.uk/11-conferences/materialscharacterisation-2011.html>

13-16 June 2011

Nanotech Conference & Expo 2011, Boston MA, USA.
<http://www.techconnectworld.com/Nanotech2011/>

13-17 June 2011

Advanced Methods in X-ray Powder Diffraction, International Centre for Diffraction Data , Newtown Square, PA, USA.
<http://www.icdd.com/education/xrd.htm>

13-17 June 2011

Resonant Elastic X-Ray Scattering, Aussois, France.
<http://rexs2011.grenoble.cnrs.fr/>

13-26 June 2011

The Zürich School of Crystallography 2011. Bring Your Own Crystals. Zürich, Switzerland.
<http://www.oci.uzh.ch/group.pages/linden/zsc/>

19-24 June 2011

Liquid Crystals, South Hadley, MA, USA.
<http://www.grc.org/programs.aspx?year=2011&program=liqucrust>

20-21 June 2011

XDL 2011 Workshop 3: Ultra-fast Science with "Tickle and Probe", Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

20-23 June 2011

I W P C P S® 13 Thirteenth International Workshop on Physical Characterization of Pharmaceutical Solids, Indianapolis, IN, USA.
http://www.assainternational.com/workshops/iwpcps_13/iwpcps_13.cfm

20-24 June 2011

XVII International Conference on Crystal Chemistry, X-ray Diffraction and Spectroscopic Studies of Minerals, St Petersburg, Russia.
<http://onlinereg.ru/ccxrds>

22-24 June 2011

Electronic Materials Conference 2011, Santa Barbara, CA, USA.
<http://www.tms.org/Meetings/Specialty/EMC11/home.aspx>

23-24 June 2011

XDL 2011 Workshop 4: High-pressure Science at the Edge of Feasibility, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

25-30 June 2011

36th Federation of European Biochemical Societies Congress, Turin, Italy.
<http://www.febss2011.it/>

26-30 June 2011

5th International Workshop on Crystal Growth Technology, Berlin, Germany.
<http://iwcg5.ikz-berlin.de/>

27-28 June 2011

XDL 2011 Workshop 5: Materials Science with Coherent Nanobeams at the Edge of Feasibility, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

29-30 June 2011

XDL 2011 Workshop 6: Frontier Science with X-ray Correlation Spectroscopies using Continuous Sources, Ithaca, NY, USA.
http://erl.chess.cornell.edu/gatherings/2011_Workshops/index.htm

30 June - 1 July 2011

European Lab Automation, including Advances in Protein Crystallography, Hamburg, Germany.
<http://www.selectbiosciences.com/conferences/APC2011/>

3-7 July 2011

iWoRID2011. International Workshop on Radiation Imaging Detectors, Zurich, Switzerland.
<http://indico.psi.ch/conferenceProgram.py?confId=29>

4-8 July 2011

Workshop on Combined Analysis Using X-ray and Neutron Scattering, Caen, France.
<http://www.inel.fr/news/page.asp?n=39>

4-8 July 2011

AIC International School 2011 Crystallography Beyond Diffraction, Camerino, Italy.
<http://www.unicam.it/geologia/AICS2011/>

4-13 July 2011

High throughput methods for protein production and crystallization, Marseille, France.
<http://events.embo.org/11-HTP/>

5-8 July 2011

UCANS-II: The Second Meeting of The Union for Compact Accelerator-Driven Neutron Sources Indiana University, Bloomington, IN, USA.
<http://www.indiana.edu/~lens/UCANS/>

9-19 July 2011

Layered mineral structures and their application in advanced technologies, Rome, Italy.
<http://www.emuschool2011.unimore.it/>

10-12 July 2011

British Association for Crystal Growth (BACG) 2011 Annual Conference held jointly with the Dutch Association for Crystal Growth (DAGC) and in partnership with the British Crystallographic Association (BCA) Industrial Group, London.
<http://www.bacg.co.uk/index.php/2011-bacg-conference>

10-15 July 2011

9th International Conference on Nitride Semiconductors, Glasgow.
<http://www.icns9.org/>

15-19 July 2011

19th Annual International Conference on Intelligent Systems for Molecular Biology & 10th European Conference on Computational Biology, Vienna, Austria.
<http://www.iscb.org/ismbeccb2011>

16-17 July 2011

Hydrogen-Metal Systems, Easton, MA, USA.
http://www.grc.org/programs.aspx?year=2011&program=grs_hydrm

17-21 July 2011

ECNS 2011. 5th European Conference on Neutron Scattering, Prague Czech Republic.
http://www.ecns2011.org/joomla_15/

17-22 July 2011

Thin Film and Crystal Growth Mechanisms. Gordon Research Conference, Biddeford, ME, USA.
<http://www.grc.org/programs.aspx?year=2011&program=thinfilm>

21 July 2011

Opening of the Barkla X-ray Laboratory of Physics Liverpool.
http://www.biophysics.liv.ac.uk/X-rays_Liverpool.html

22-23 July 2011

S&S@ess conference, Prague, Czech Republic.
<http://ess-scandinavia.eu/s-and-s>

24-29 July 2011

Clusters, Nanocrystals & Nanostructures, South Hadley MA, USA.
<http://www.grc.org/programs.aspx?year=2011&program=clusters>

31 July - 5 August 2011

18th American Conference on Crystal Growth and Epitaxy in conjunction with the 15th US Biennial Workshop on Organometallic Vapor Phase Epitaxy, Monterey, CA, USA.
<http://crystalgrowth.us/accge18/index.php>

1-5 August 2011

DXC 2011. 60th Annual Denver X-ray Conference, Denver, CO, USA.
<http://www.dxcicdd.com/>

1-5 August 2011

THERMEC-2011 - Neutron Scattering & X-Ray Studies of Advanced Materials, Quebec, QC Canada.
<http://www.thermec2011.ca/>

1-5 August 2011

10th International Conference on the Structure of Surfaces and e-ICSOS-10, Hong Kong, China.
<http://icsos10.ap.cityu.edu.hk/>

7-12 August 2011

X-ray Science. Gordon Research Conference, Waterville, ME, USA.
<http://www.grc.org/programs.aspx?year=2011&program=xray>

13-22 August 2011

10th PSI Summer School: Probing Phase Transitions using Photons, Muons and Neutrons, Zug, Switzerland.
<http://indico.psi.ch/conferenceDisplay.py?confId=258>

16-22 August 2011

Mieres 2011: Crystallographic Computing School, Oviedo, Spain.
<http://www.iucr.org/resources/commissions/crystallographic-computing/schools/mieres2011>

20-21 August 2011

Categorizing Halogen Bonding and Other Noncovalent Interactions Involving Halogen Atoms, Sigüenza, Guadalajara, Spain.
<http://www.iucr2011madrid.es/index.php/program/satellite-meetings>

22-29 August 2011

IUCr2011. XXII Congress and General Assembly, Madrid, Spain.
<http://www.iucr2011madrid.es/>

30 August – 1 September 2011

Crystallography of Hispano-Islamic Ornamental Art: Visit to the Alhambra, Granada, Spain.
<http://www.iucr2011madrid.es/index.php/program/satellite-meetings>

31 August - 1 September 2011

Aperiodic Crystals for Beginners: satellite meeting to the Madrid 2011 XXII IUCr Congress, Alcala de Henares, Spain.
<http://sig3.ecanews.org/aperbeg2011/aperbeg2011.html>

31 August - 3 September 2011

Online Edition of International Tables for Crystallography: Current State and Future Developments Bilbao Spain
http://www.iucr.org/news/notices/meetings/meeting_2011_ps_01

30 August - 4 September 2011

International School on Charge Density, Jaca, Spain.
<http://www.iucr2011madrid.es/index.php/program/satellite-meetings>

1-2 September 2011

9th International NCCR Symposium on New Trends in Structural Biology, Zurich, Switzerland.
<http://www.structuralbiology.uzh.ch/index.php?q=node/105>

4-7 September 2011

ECMS2011. 7th European Conference on Mineralogy and Spectroscopy, Potsdam, Germany.
<http://www.physchemgeo.com/ECMS/>

4-8 September 2011

Diamond 2011. 22nd European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes and Nitrides, Garmisch-Partenkirchen, Germany.
<http://www.diamond-conference.elsevier.com/index.html>

4-9 September 2011

24th European Conference on Biomaterials, Dublin, Ireland.
<http://www.esb2011.org/>

5-16 September 2011

12th Oxford School on Neutron Scattering St. Anne's College, University of Oxford
<http://www.oxfordneutronschool.org/>

6-9 September 2011

MECA SENS VI: 6th International Conference on Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation, Hamburg, Germany.
<http://www.mecasens2011.de/>

11-14 September 2011

Recent Advances in Macromolecular Crystallization, Le Bischenberg, Strasbourg, France.
<http://www.tcp-events.co.uk/ramc2011/>

13-16 September 2011

ISIC18. 18th International Symposium on Industrial Crystallization, Zürich, Switzerland.
<http://www.isic18.ethz.ch/>

18-22 September 2011

DyProSo XXXIII. 33rd International Symposium on Dynamical Properties of Solids, Aussois, France.
<http://www.ill.eu/news-events/events/dyproso-xxxiii/home/>

4-7 October 2011

Trends and Perspectives in Neutron Instrumentation: From Continuous to Spallation Sources, Tutzing, Germany.
http://www.jcns.de/Workshop_2011

11-13 October 2011

Handheld XRF Workshop, International Centre for Diffraction Data, Newtown Square, PA, USA.
<http://www.icdd.com/education/handheld-xrf-workshop.htm>

12-14 October 2011

ADD 2011. Workshop on Analysis of Diffraction Data in Real Space, Grenoble, France.
<http://www.ill.eu/news-events/events/add2011/>

17-19 October 2011

Basic Rietveld Refinement & Indexing, International Centre for Diffraction Data, Newtown Square, PA, USA.
<http://www.icdd.com/education/rietveld-workshop.htm>

20-21 October 2011

Advanced Rietveld Refinement & Indexing, International Centre for Diffraction Data, Newtown Square, PA, USA.
<http://www.icdd.com/education/rietveld-workshop.htm>

8-11 November 2011

9th TOPAS Users' Meeting with hands-on sessions, Bad Herrenalb, Germany.
http://www.bruker-axs.com/topas_users_meeting_2011.html

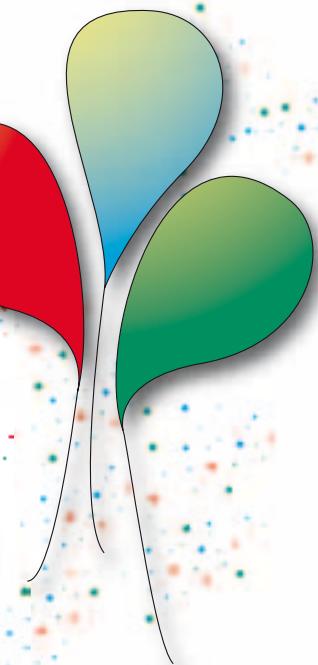
25-29 August 2013

28th European Crystallographic Meeting, University of Warwick.
<http://www.crystallography.org.uk/>

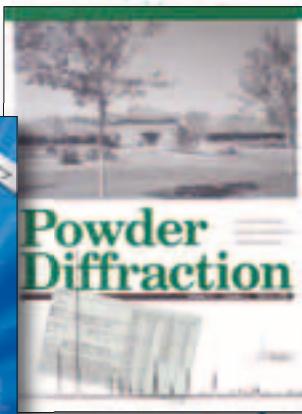
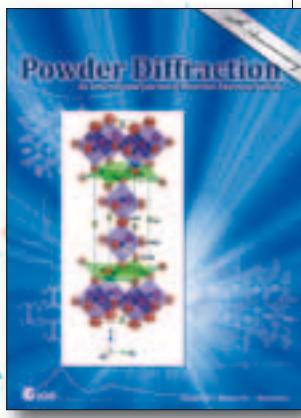
International Centre for Diffraction Data

Celebrating

70th Anniversary
Serving the
Scientific
Community



25th Anniversary
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Powder Diffraction



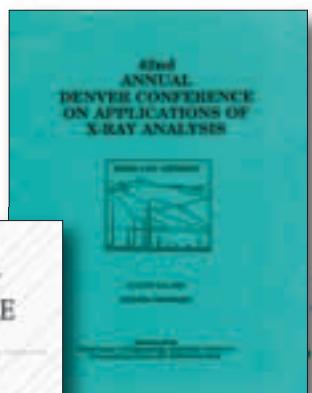
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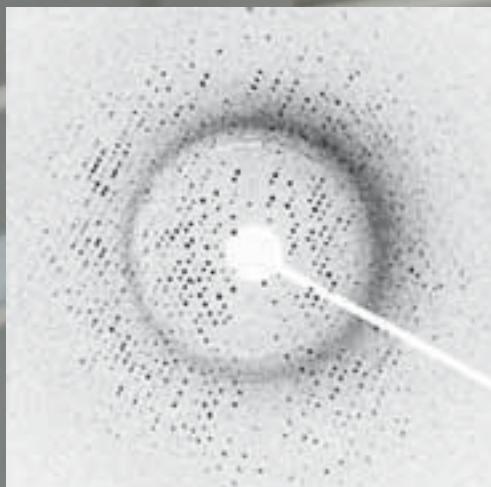
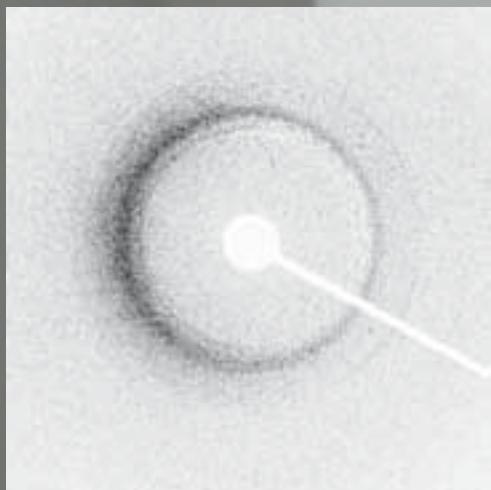


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60th Anniversary
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Denver
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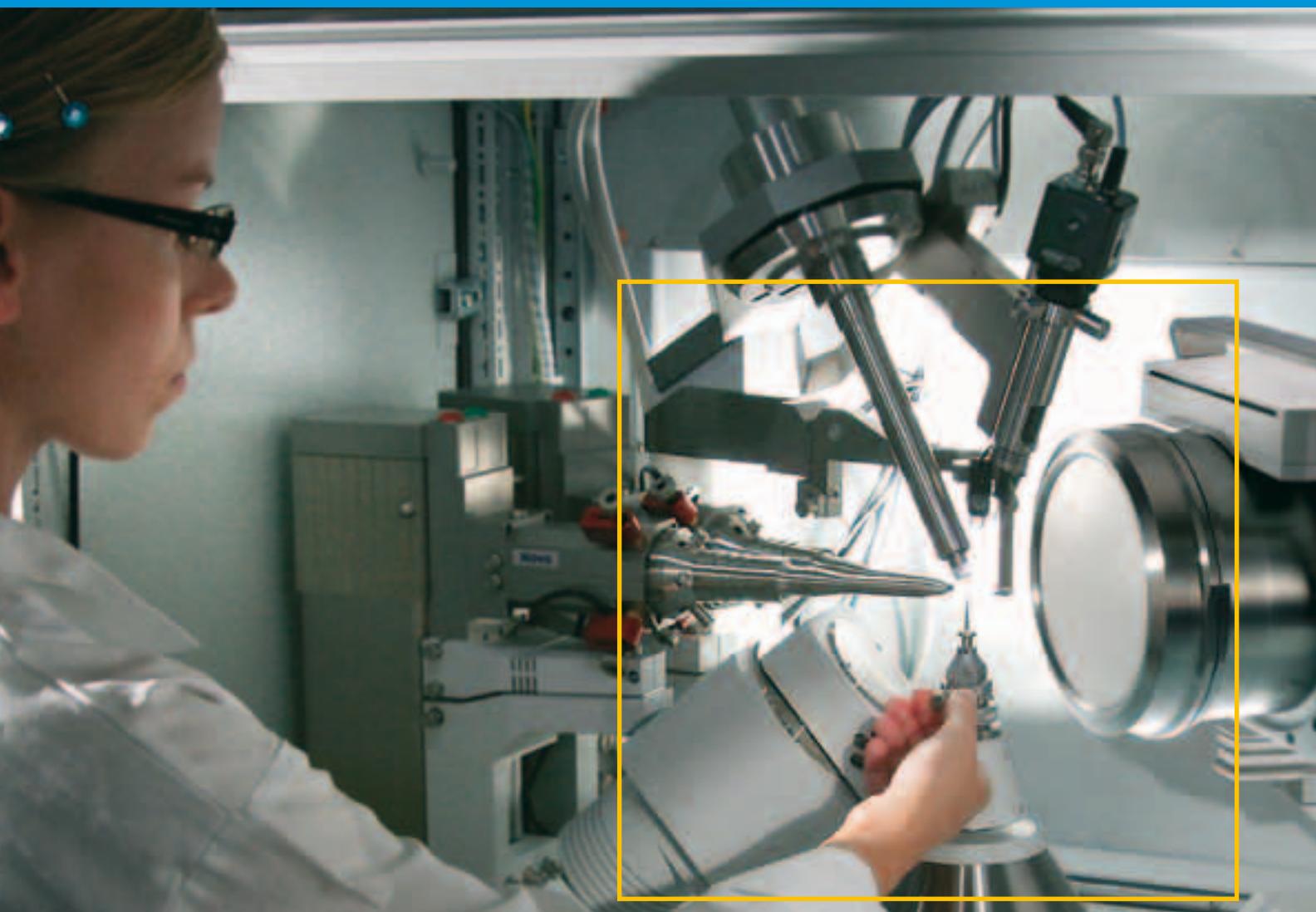


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Open flow LN₂ cooler: 80-500 K

Cobra & Cobra Plus
Non-liquid nitrogen cooler: 80-500 K

N-HeliX
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Desktop Cooler
Compact non-liquid cooler: 170-290 K

Phenix
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That's all we do. Why?

Well, we believe that being entirely focused on one area of expertise, allows us to develop and manufacture the most advanced, reliable and easy-to-use range of coolers available for X-ray crystallography.

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